UPGRADING PHYSICS PACKAGES FOR LAHET™ /MCNPX™

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ABSTRACT

A number of the physics capabilities have been upgraded in the developmental version of LAHET for the eventual use in MCNPX. These include a high-energy generator for particle interactions, complete definition for particle reaction and elastic scattering cross sections, a current mass excess tabulation, and an improved stopping power formulation. These developments are reported in this paper, along with some identification of the areas of continuing effort.

I. INTRODUCTION

Code development efforts in support of APT and proton radiography[1] require the upgrade of the various physics packages in LAHET[2] and, through code merger, in MCNPX.[3] In some cases, the end product is a new capability. In others, the result is a general improvement and updating of existing capabilities, perhaps with the introduction of new computational methods. In any case, testing and documentation of the various physics packages is part of the ongoing quality assurance program for the development of MCNPX.

The particular topics that are discussed here are the following:

1. the adaptation of the FLUKA96 high-energy generator to extend the MCNPX transport capability to energies above 1 TeV;
2. the implementation of a procedure to provide defined reaction and elastic scattering cross sections for all particles in LAHET and, in the absence of nuclear data libraries, in MCNPX;
3. the development of a new atomic mass data base and the code to access it for all the physics packages shared by LAHET and MCNPX;
4. the construction of a stopping power generator that is much improved over the original method used in earlier LAHET versions for the transport of all particles with mass greater than or equal to the muon.

At the present time, the stopping power method has been implemented in MCNPX as well as the developmental version of LAHET (LAHET3). The other developments have been tested in LAHET3 and should be implemented in MCNPX later this year. A more extensive discussion of the general MCNPX code development effort may be found elsewhere in these transactions.[4]

II. HIGH ENERGY PHYSICS CAPABILITY

To provide a high energy computational capability, the high-energy generator from FLUKA96[5] has been coupled to the existing Bertini and ISABEL intranuclear cascade models. The result is a much-improved model for nucleons and pions above 3.5 GeV and a new interaction capability for kaons and antinucleons above 1 GeV. Applications of the new feature have been reported in reference 1. The transition between the FLUKA96 module and the Bertini internuclear cascade model may be set at any incident energy above 500 MeV, or the transition may be defined by random linear interpolation over an energy range. For particles that must use the ISABEL INC for interaction at lower energies, the transition between models is nominally set at 1 GeV, 800 MeV for kaons. The cross section definition subroutines from FLUKA96 were included in the FLUKA96 code segment implemented in LAHET3. Their application is discussed in the next section.

III. CROSS SECTION DEFINITION

In earlier versions of LAHET, as in HETC and other intranuclear cascade codes, reaction cross sections are not predetermined, but are rather implicitly determined by the models. In the new approach developed for LAHET3 and MCNPX, total reaction and elastic scattering cross sections are fully defined and represented by parameterizations and tabulations. Even in a preliminary form, this approach has shown previously significant improvement in comparisons of calculations with medium-energy benchmark experiments[6]. Both optical model cross sections[7] and cross sections parameterized from experimental data [5,8,9] are employed. At lower energies, compatibility with the new MCNPX 150 MeV nucleon libraries can be maintained.

An algorithm has been constructed to provide the definition of the reaction cross section (σ_R) and the elastic scattering cross section (σ_{el}) for all transported particle types interacting with any target (Z,A) at all energies. The current algorithm, provisional in nature, has the following features:

1. the *default* procedure, used in the absence of any other criterion, obtains σ_R and σ_{el} from the FLUKA96 models;
2. for *nucleons* on targets with A > 4, σ_{el} (only) is defined by the model previous implemented in LAHET2.8;[7]
3. for *pions* below 40 MeV, both σ_R and σ_{el} are obtained by the methods of Barashenkov and Polanski;
4. for *antinucleons* below 51 MeV, the cross sections are held constant by their value at 51 MeV;
5. for *ions* (d, t, ^{3}He, α), σ_R is obtained by the NASA[8] methods and $\sigma_{el} \equiv 0$.

As noted, the above procedure is subject to continuing development. Current efforts are directed toward

1. using tabulated data from the 150 MeV MCNPX neutron and proton data libraries;
2. using tabulated optical model calculations to 400 MeV for nucleons on such targets as are appropriate;
3. selectively integrating the available parameterization methods based on the studies reported in reference 10.

However, now that the interface to the cross section definition procedure is defined, the MCNPX development effort may focus on developing the logic for nucleon transport in materials where some isotopes may have reactions defined by the 150 MeV MCNP-type data libraries and others are treatable only by the above cross section algorithm and LAHET-type interaction physics.

IV. MASS DATA TABLES

A common atomic and nuclear mass excess tabulation has been constructed for use by all medium- and high-energy physics modules; the implementation included removal of all ^{16}O-scale mass usage in the oldest code segments. In constructing the tabulation, the experimental mass data of Audi and Wapstra[11] are extended with the calculations of Möller *et al.*[12] Extrapolation even farther from stability was obtained by using the spherical form of the finite-range droplet model (FRDM).[12] Continuity was insured by matching the FRDM extrapolation to the last available "known" (experimental or calculated) mass along a line of constant charge (for neutron-rich nuclei) or along a line of constant neutron number (for proton-rich nuclei). Thus, for $N > N_0$, the extrapolated mass excess $\tilde{X}(Z,N)$ is

$$\tilde{X}(Z,N) = F(Z,N) - F(Z,N_0) + X(Z,N_0)$$

where $X(Z,N_0)$ is obtained from reference 10 or 11, and $F(Z,N)$ is the form of the spherical FRDM from reference 11.

The motivation for the effort was not only to update the mass excess data but to improve estimation far from the lines of stability. The latter is necessary since the intranuclear cascade calculation may produce intermediate state residual nuclei very far from the lines of stability. It is not impossible for an INC calculation to produce an intermediate state such as

$$p + {}^{12}C \rightarrow {}^{6}C + p + 6n$$

with the subsequent deexcitation through an evaporation or breakup model of the intermediate state ${}^{6}C \rightarrow 6p$. The mass excess data used in such a sequence must allow the disintegration process to continue to a plausible final outcome.

In constructing the data tables for Z $\geq$ 8 and N $\geq$ 8, 1888 experimental masses from the Audi/Wapstra "experimental" file were included and supplemented with 4756 additional calculated values.[12] For Z < 8 or N < 8, 87 values were obtained from the Audi/Wapstra "recommended" file. An additional 14 suppositional mass excess values, for light nuclei far from stability and previously used with the LAHET Fermi breakup model, were added. Since the table structure allows up to 41 entries for each mass value A, the spherical FRDM was used to fill remaining table entries.

A comparison of the calculated[12] values with the experimental tabulation for the 1888 nuclei with $Z \geq 8$ and $N \geq 8$ shows a mean deviation of 0.016 MeV and an RMS deviation of 0.69 MeV. A similar comparison of the spherical FRDM with experiment indicates a mean deviation of 0.11 MeV and an RMS deviation of 3.32 MeV; a comparison for the 87 experimental values for Z < 8 or N < 8 shows a mean deviation of 0.71 MeV and an RMS deviation of 6.29 MeV. It was determined during testing that the extrapolation procedure, based on the spherical FRDM as described above, produced mass excess values for unstable light nuclei which are at least *numerically* acceptable, even down to Z = 0 or N = 0.

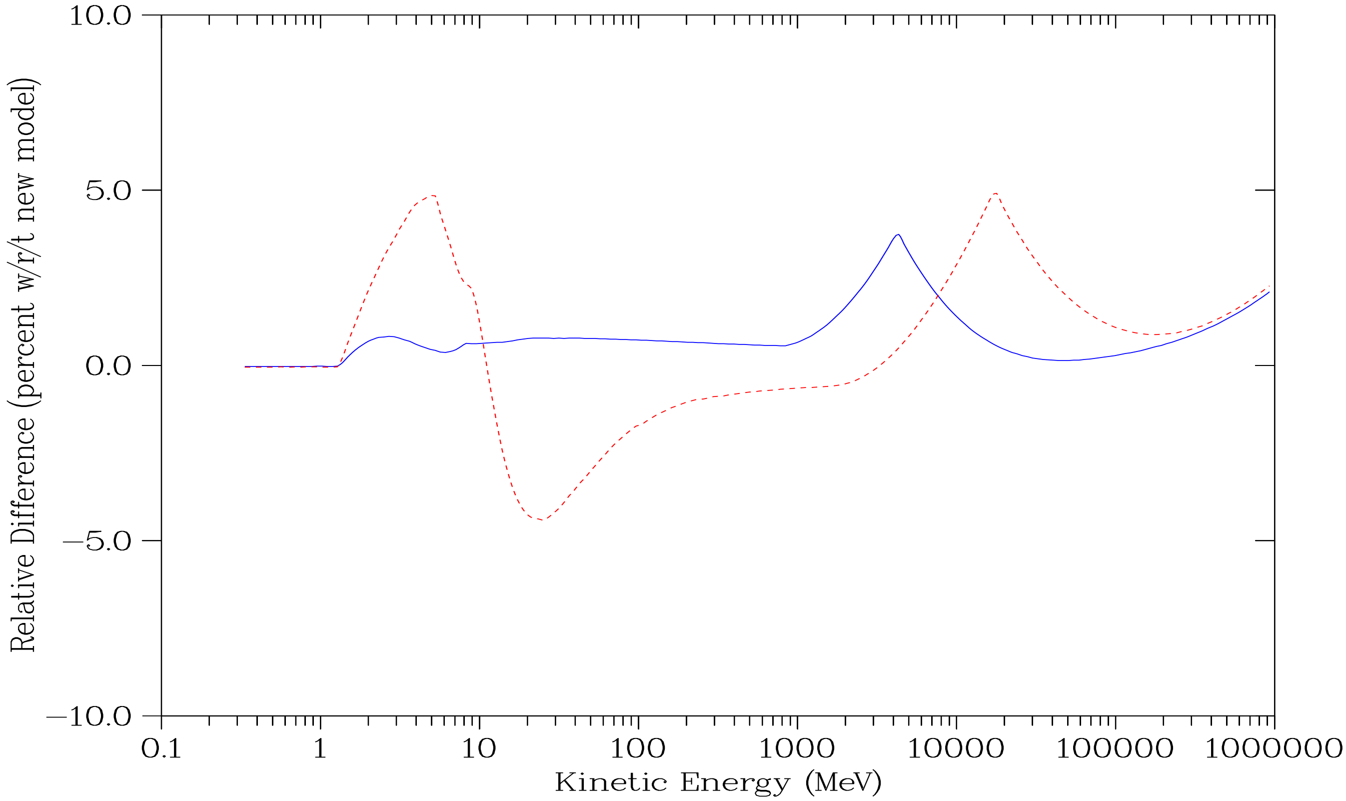

Figure 1: Relative difference of the SPAR stopping power model to the enhanced model implemented in MCNPX. The *solid* line is for protons in water; the *dashed* line is for protons in ^{238}U.

V. STOPPING POWER METHODS

A common stopping power method has been implemented in both LAHET3 and MCNPX. All earlier versions of LAHET have used the stopping power methodology implemented in the original HETC.[13] The latter was obtained from the ORNL SPAR code.[14] In the new implementation, the low-energy method has been left unchanged from SPAR usage for particle energies below 1 MeV/AMU. However, for incident energies above 1 MeV/AMU, the coding has been fully rewritten to provide more accurate results for our current programmatic needs. Undesirable approximations have been removed at high energies and better approximations for corrections terms to the Bethe-Bloch formula have been used to improve on the treatment originally used for LAHET. At some future date, we intend to upgrade the low-energy modeling, perhaps using features from the LARC code recently developed by NASA.[15]

All the kinematic terms have been retained in our implementation of the Bethe-Bloch formula. The full relativistic expression for the maximum kinetic energy transfer to an unbound electron at rest is used. The common approximation of neglecting the ratio of the electron mass to the incident particle mass has **not** been made; the latter approximation appears in both SPAR and LARC. In figure 1, the relative difference between the original (SPAR) method and the new implementation is shown. The elimination of the above approximation is reflected in the increasing discrepancy above 100 GeV; it significant well below 10 GeV for muons and pions.

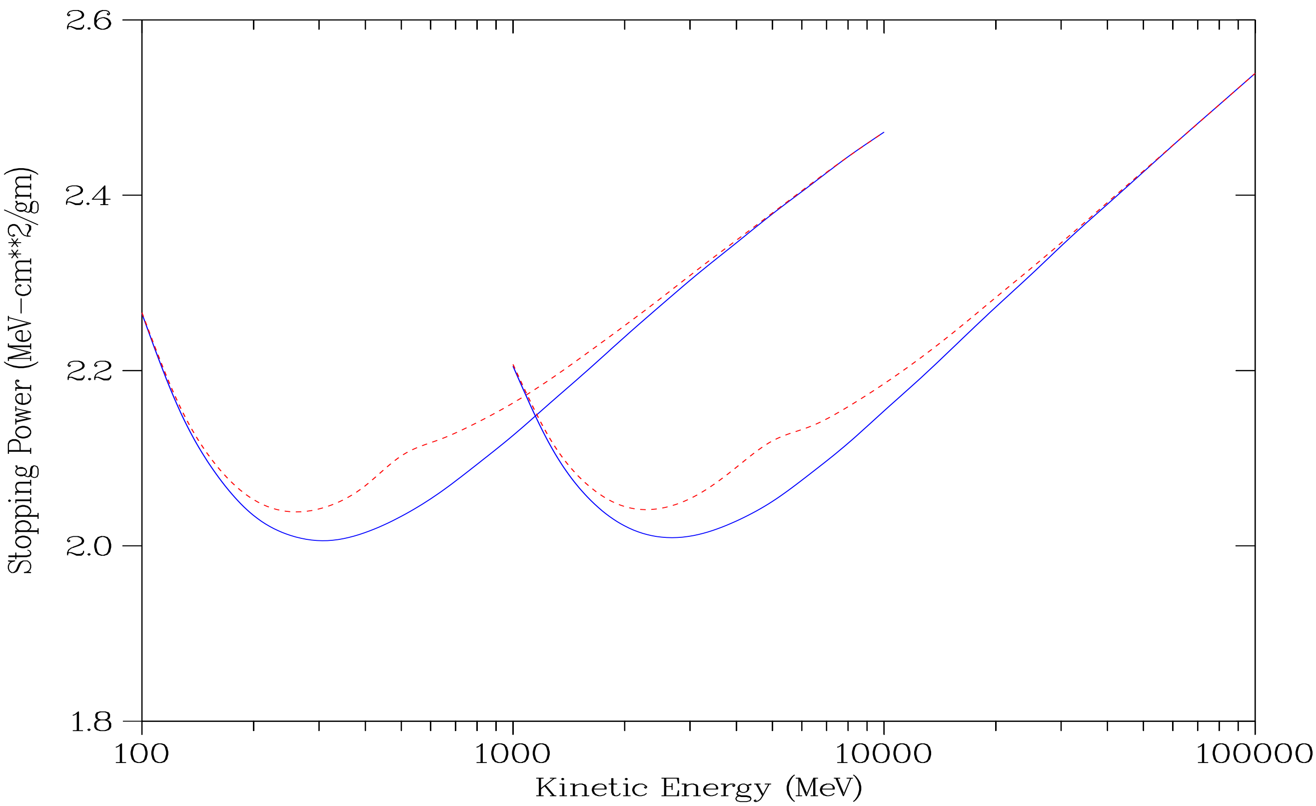

Figure 2: Comparison of the "asymptotic" form (*dashed* line) of the density effect correction to the full method (*solid* line). Muons in water are shown by the curves at the left, protons in water by the curves at the right.

The Sternheimer-Peierls density effect correction[16] to the Bethe-Bloch formula appears in the SPAR methodology in the often used "asymptotic" form. In the new package, it is used in its "full" specification as appears in the MCNP treatment for electrons. The difference between the two approaches may be quite significant, as shown in figure 2; the strange peak in the curve is an artifact that arises from the use of the asymptotic form. The peak is also noticeable in the difference curve in figure 1. The effect is most significant at a few GeV for protons and below a GeV for muons.

The shell correction (C/Z) to the Bethe equation that is used is adapted from Janni.[17] This term is significant below 100 MeV/AMU for high-Z materials and at only at much lower energies for low-Z materials. In figure 1, the change in method is most obvious for the ^{238}U case at low energies.

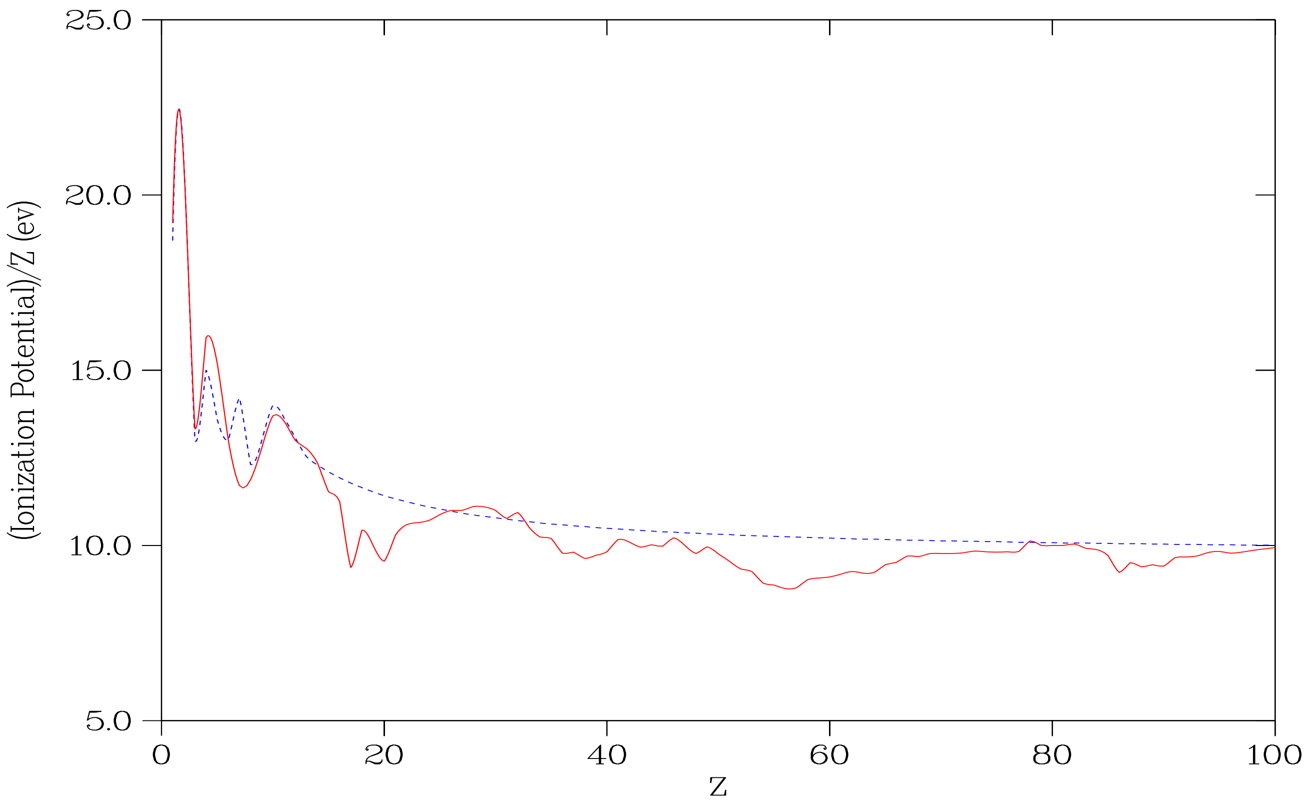

Figure 3: Ionization potentials from ICRU37[18] are shown in *solid line*. Ionization potentials from SPAR[14] are shown in the *dashed* line. The former is included in the new LAHET3/MCNPX implementation.

The ionization potentials employed are those recommended in ICRU Report 37.[18] The values are dependent on whether the element is pure or in a mixture. The ionization potential for light isotopes is also dependent on gaseous or condensed state. A comparison of the ionization potential adapted from ICRU37 (pure element, natural state) with values formerly used in LAHET with the SPAR model are shown in figure 3.

A number of other correction terms to the Bethe-Bloch formula are discussed (and dismissed) in reference 15. The second-order Born approximation correction discussed in reference 17, never larger than a few tenths of a percent, is included for compatibility with Janni.

VI. CONCLUSIONS

Following our approach to the code merger[3], the above methods have been tested in the developmental LAHET3. The new physics upgrades are or will be included in future releases of MCNPX, where they will complement the many other aspects of the code development.[4]

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